

Tryptophan, MTH-TMS

Inchi: InChI=1S/C19H29N3OSSi2/c1-21-18(23-26(5,6)7)16(20-19(21)24)12-14-13-22(25(2,3)4)
InchiKey: QBRRWSVRCYUTBE-UHFFFAOYSA-N
Formula: C19H29N3OSSi2
SMILES: Cn1c(O[Si](C)(C)C)c(Cc2cn([Si](C)(C)C)c3ccccc23)[nH]c1=S
Mol. weight [g/mol]: 403.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	5.043		Crippen Method
rinpol	2631.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525525&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/68-171-7/Tryptophan-MTH-TMS.pdf>

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